Automating Life Detection Using Lipid Detection in GCMS Data

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NASA SILICON VALLEY
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Shell

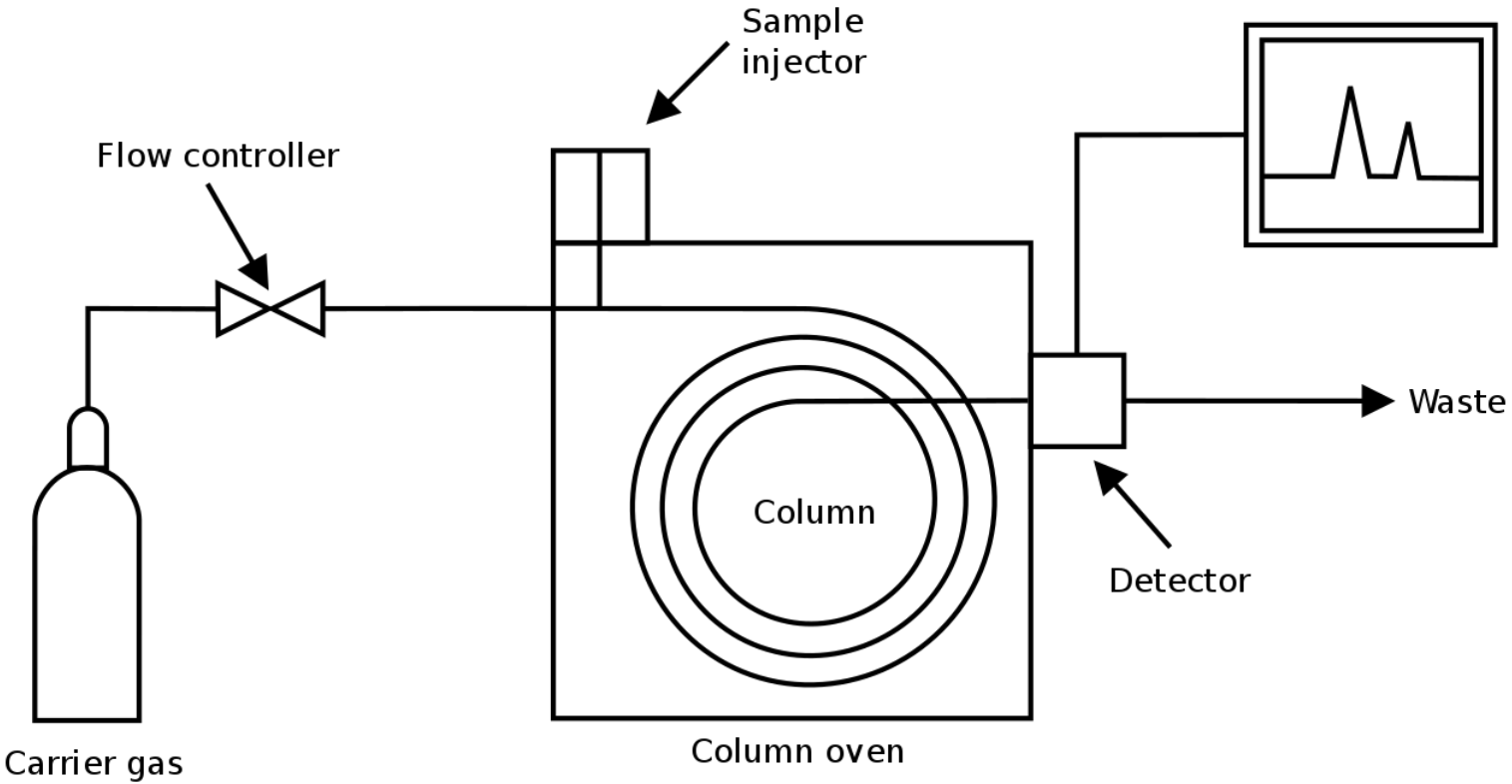
rough draft of project patch!

ExCALiBR

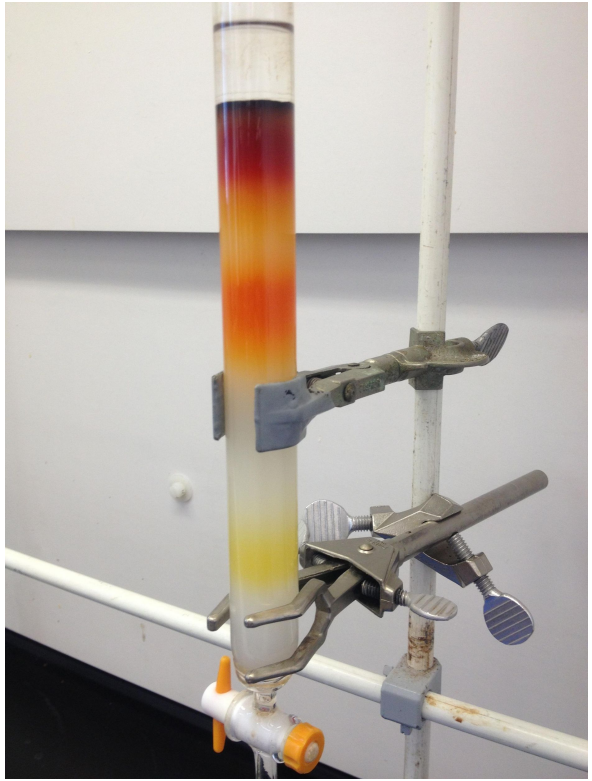
Extractor for **C**hemical **A**nalysis of **Li**pid **B**iomarkers in **R**egolith

1. Building an instrument to extract and purify lipids from regolith to enable optimal GC-MS analysis.
2. Automatically classify lipids as being of ***biotic*** or ***abiotic*** origin.
3. Predict processing parameters for follow-on sampling and sample processing.

Gas Chromatography



Chromatogram



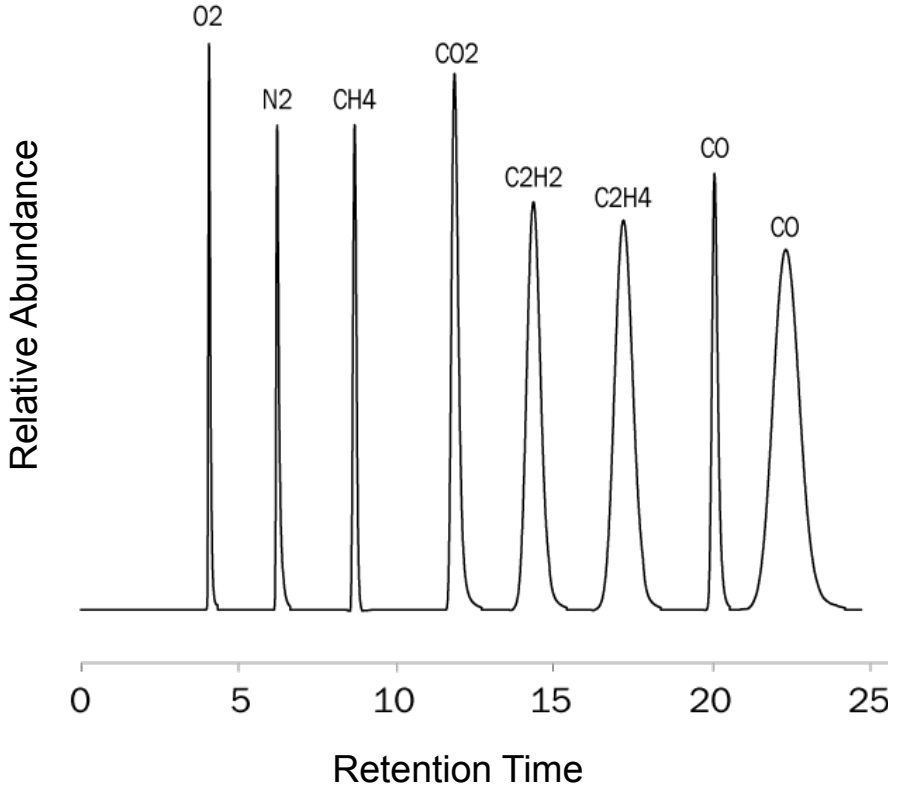


Image source: LDetek

Mass Spectrometry

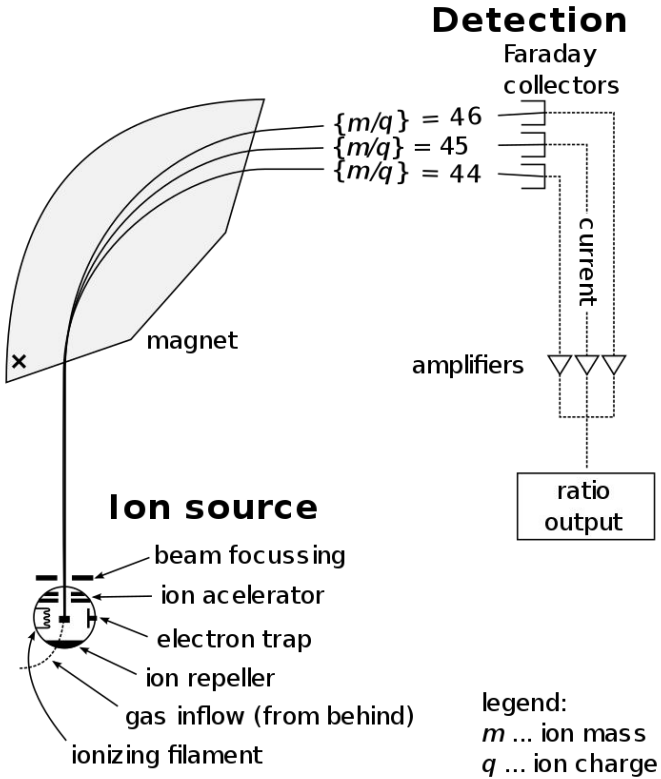


Image source: US Geological Survey via Wikipedia

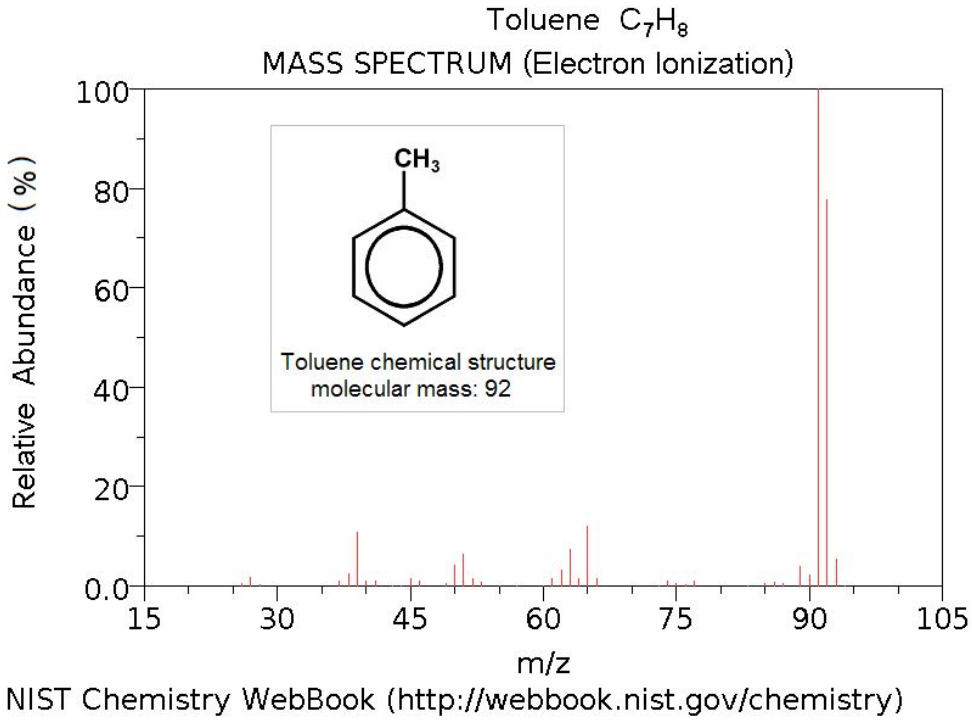


Image source: US Government-NIST via H. Padleckas

Gas Chromatograph - Mass Spectrometer

- Combines both modalities to yield more information about samples.
- Amenable to operations on other planetary bodies.
- Good at detecting organic molecules that tell us about life (e.g. ***lipids***)

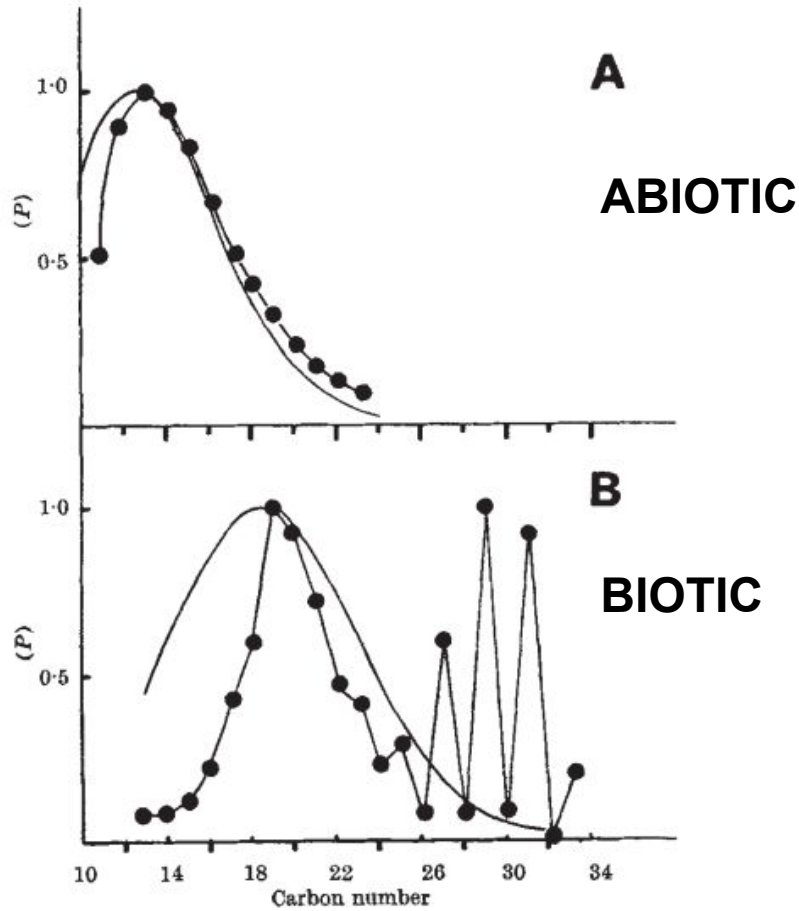
Why Lipids?

Changes the question from:

Can organisms live here?

to:

Does this sample contain an organism?



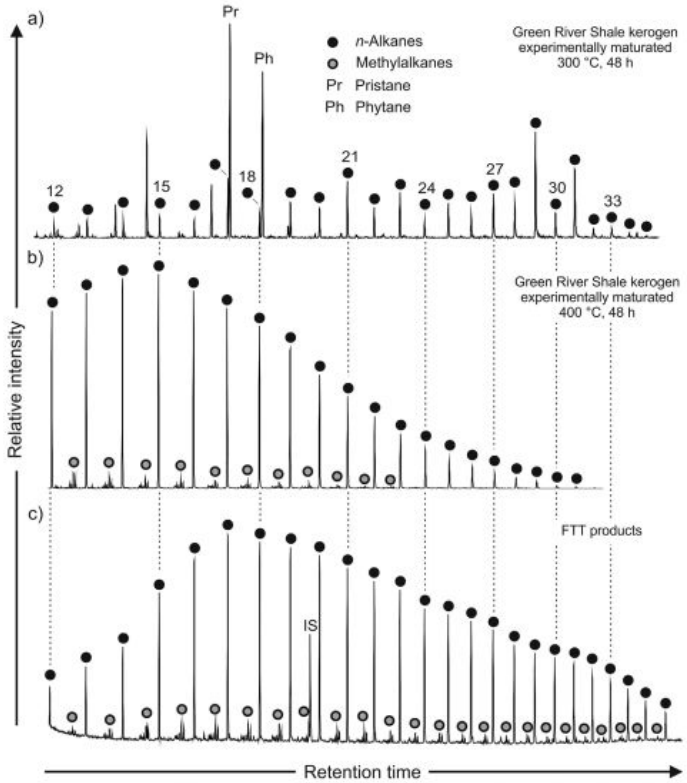
Source: *A Physical Basis for Life Detection Experiments*, Lovelock, Nature #4995 (1965)

Can We Classify Origin Process for Lipids?

BIOTIC

ANCIENT BIOTIC

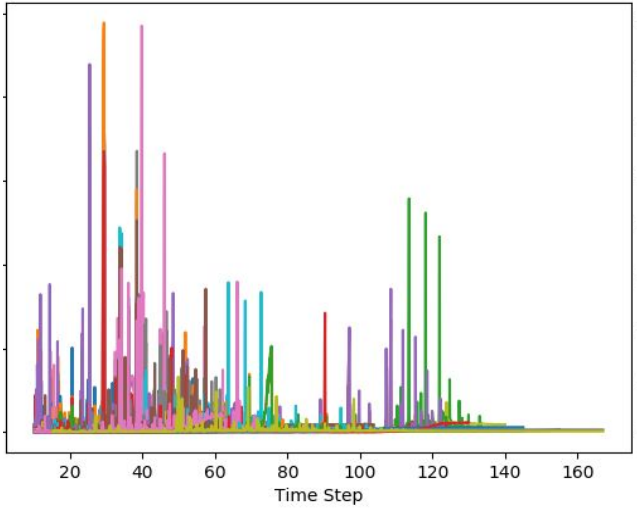
ABIOTIC



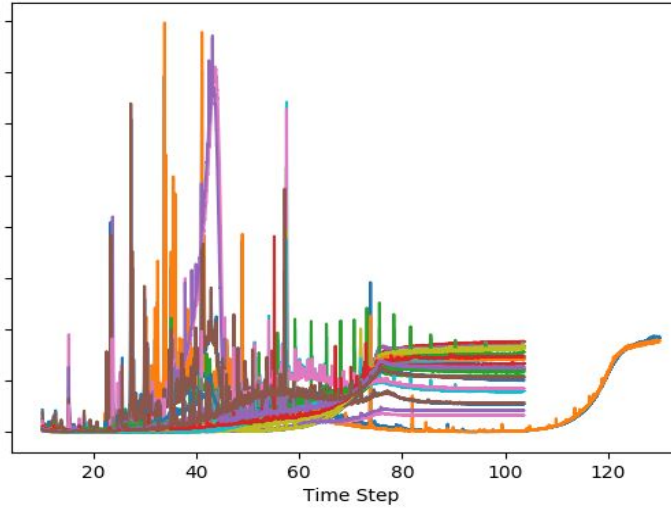
- Not just looking for lipids in old places.
- Geological processes can transform signature of materials of ***biotic*** origin to look like materials of ***abiotic*** origin.

Source: *Assessing the diversity of lipids formed via Fischer-Tropsch-type reactions* Mißbach *et al.*, Organic Geochemistry 119 (2018)

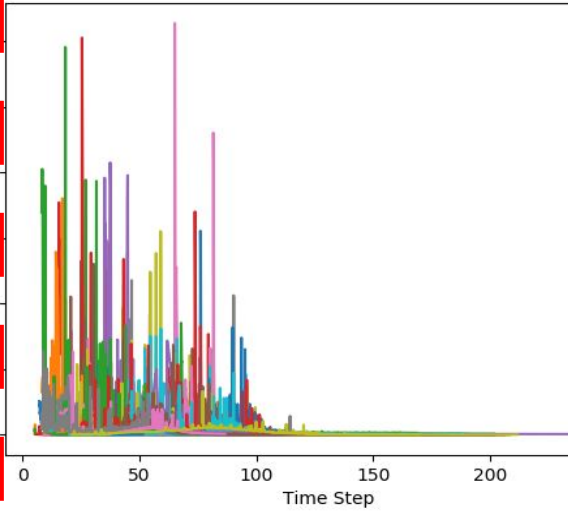
Can We classify Origin Process for Lipids?



BIOTIC

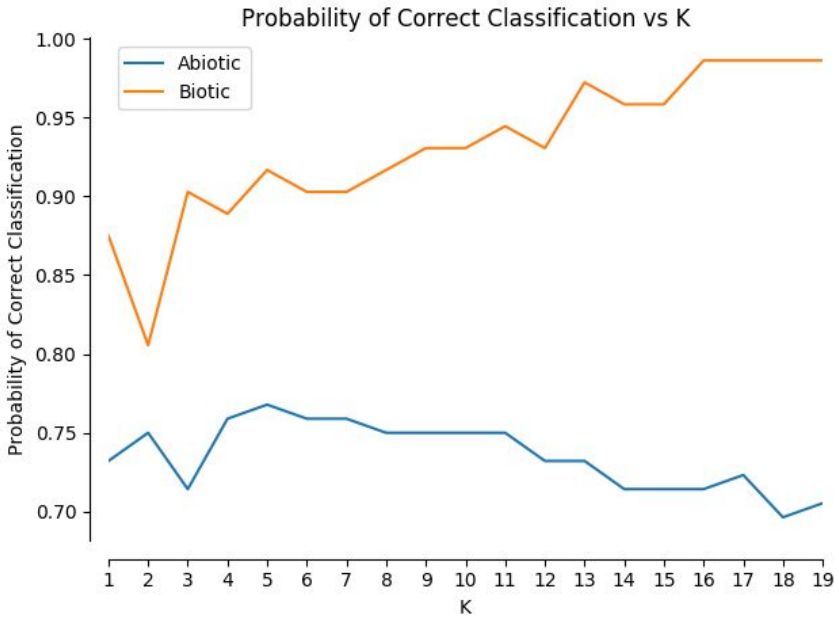


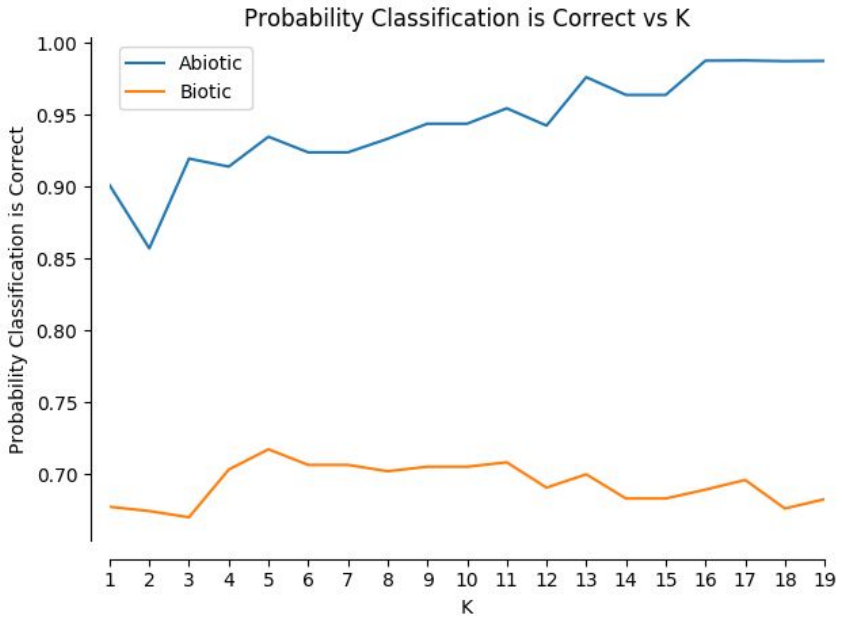
ANCIENT BIOTIC



ABIOTIC

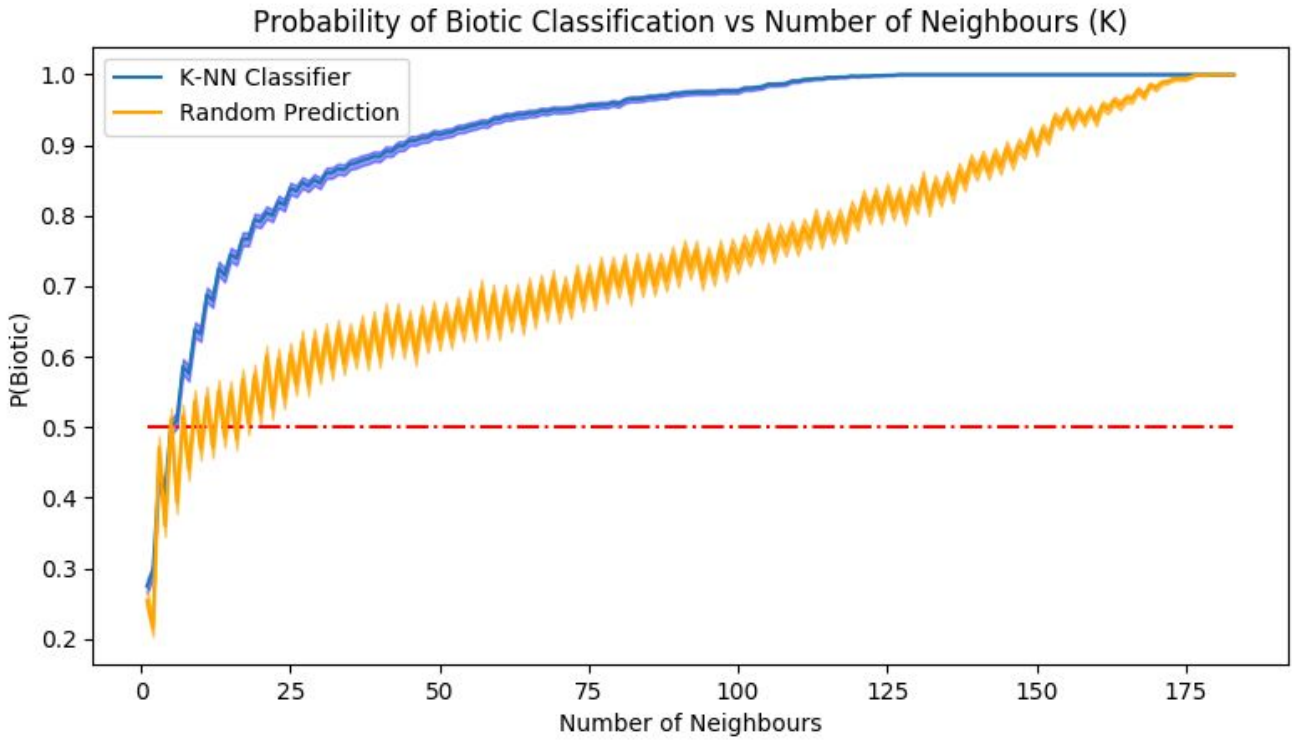
Preliminary Results: Yes





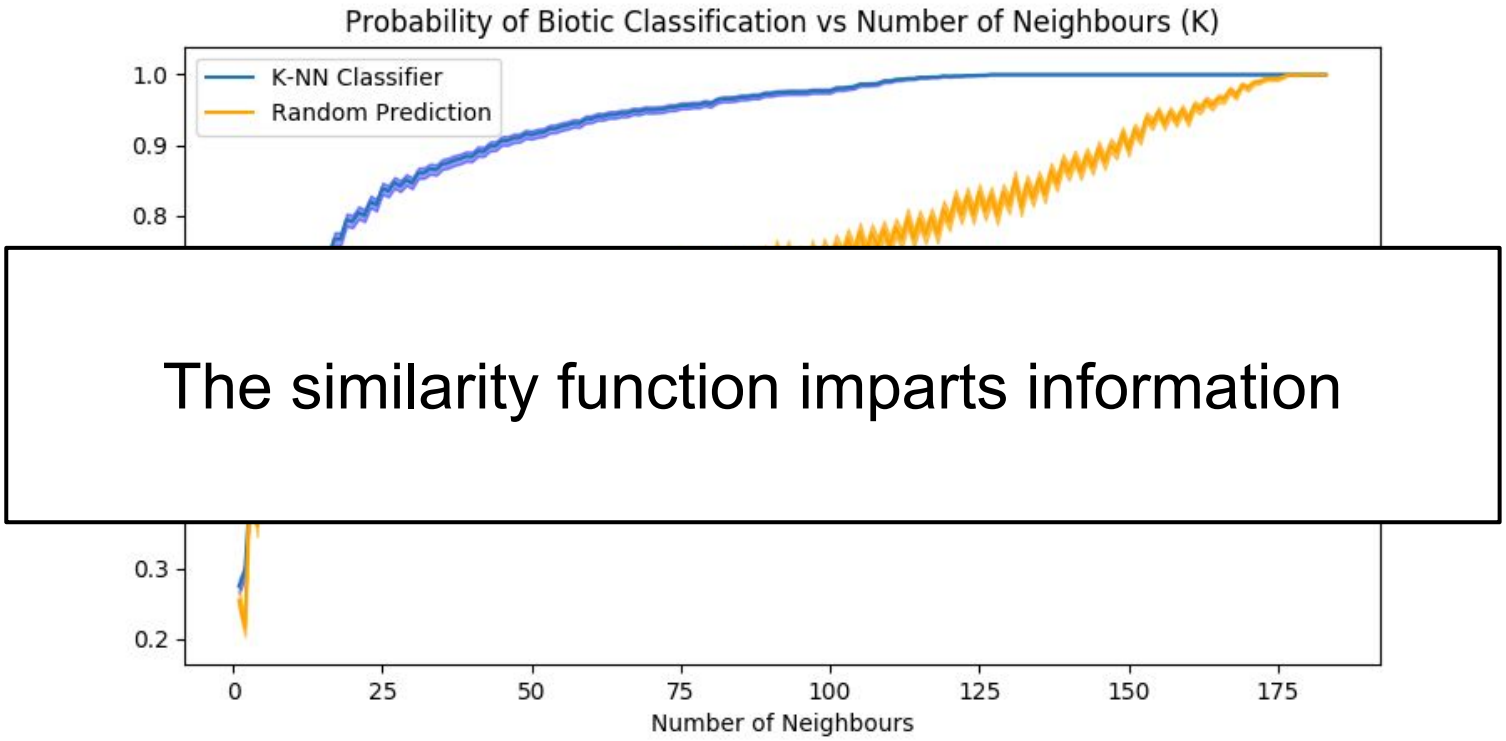
Leave-one-out validation results using K-Nearest Neighbour Classifier

More thrilling results!



Classification of 1931 ***biotic*** samples.

More thrilling results!



The similarity function imparts information

Classification of 1931 ***biotic*** samples.

Continuing Steps

- Improving Dataset quality
  - Existing dataset represents multiple decades of collection.
  - Abiotic samples are exceedingly rare.
- Considering alternative representations of GCMS data

Questions?